Ref #	Hits	Search Query	DBs	Default Operator	Plurals	Time Stamp
L1	1	("5698401").PN.	USPAT	OR	OFF	2005/09/29 18:13
L2	1	("5804390").PN.	USPAT	OR	OFF	2005/09/29 18:19
L8	168022	NMR OR (nuclear adj magnetic adj resonance)	US-PGPUB; USPAT; EPO; JPO; DERWENT	OR	ON	2005/09/29 18:22
L9	2179	l8 with ligand	US-PGPUB; USPAT; EPO; JPO; DERWENT	OR	ON	2005/09/29 18:22
L10	587	l9 with (protein OR polypeptide OR (amino adj acid))	US-PGPUB; USPAT; EPO; JPO; DERWENT	OR	ON	2005/09/29 18:23
L11	197	l10 with label$3	US-PGPUB; USPAT; EPO; JPO; DERWENT	OR	ON	2005/09/29 18:23
L12	9	l11 with (method OR process)	US-PGPUB; USPAT; EPO; JPO; DERWENT	OR	ON	2005/09/29 18:25
L13	5	l11 with spectrum	US-PGPUB; USPAT; EPO; JPO; DERWENT	OR	ON	2005/09/29 18:25
S1	16	maurizio near2 pellecchia	US-PGPUB; USPAT; EPO; JPO; DERWENT	OR	ON	2005/09/29 18:13

(FILE 'HOME' ENTERED AT 19:27:48 ON 29 SEP 2005)

FILE 'MEDLINE, EMBASE, BIOSIS, CAPLUS' ENTERED AT 19:28:39 ON 29 SEP 2005
L1 608015 S NMR OR (NUCLEAR MAGENTIC RESONANCE)
L2 15224 S L1 (S) LIGAND
L3 1435 S L2 (S) (PROTEIN OR POLYPEPTIDE OR (AMINO ACID))
L4 122 S L3 (S) LABEL?
L5 24 S L4 (S) (METHOD OR PROCESS OR USE)
L6 19 S L4 (S) SPECTRUM
L7 14 DUP REM L5 (10 DUPLICATES REMOVED)
L8 7 DUP REM L6 (12 DUPLICATES REMOVED)

AU Evers, Alex S.; Dubois, Brian W.; Burris, Kimberley E.
SO Progress in Anesthetic Mechanism (1995), 3(Proceedings of the International Workshop on Anesthetic Mechanisms, 1994), 151-7
CODEN: PAMEF6; ISSN: 0919-6390
TI Saturable binding of volatile anesthetics to proteins studied by 19F-NMR spectroscopy and photoaffinity labeling
AB While the mol. mechanism(s) of volatile anesthetic action remains unknown, indirect evidence suggests that volatile anesthetic binding to specific protein sites may underlie anesthetic action. We have employed two methods, 19F-NMR exchange spectroscopy and photoaffinity labeling with [3H]-halothane, to directly examine anesthetic binding to several proteins that contain binding sites for hydrophobic ligands. NMR and affinity labeling studies both demonstrated fatty acid-displaceable binding of halothane to serum albumin and to four fatty acid binding proteins (FABPs) that we have examd.; the affinity of halothane binding to these proteins varied over a wide range (intestinal FABP KD >>10 mM, albumin KD = 0.7 mM) suggesting structurally specific interactions of halothane with fatty acid binding sites. Consistent with structural specificity, a mutation in the fatty acid binding site of intestinal FABP (Arg106-Thr) reduced the KD for halothane to 5.1 mM. NMR and affinity labeling studies also demonstrated saturable binding (KD = 0.7 mM) of halothane to firefly luciferase. Halothane labeling of luciferase was reduced by a luciferin analog, but not by other volatile anesthetics; this result suggests that volatile anesthetics do not compete for a common binding site on firefly luciferase. In summary, this paper demonstrates methods for directly studying volatile anesthetic binding to proteins and suggests that a variety of proteins are likely to bind volatile anesthetics at clin. relevant concns.

IN Fesik, Stephen W.; Hajduk, Philip J.
SO PCT Int. Appl., 52 pp.
CODEN: PIXXD2
TI Use of 13C-NMR to detect binding
AB Methods of detecting binding of a putative ligand to a 13C-enriched target mol., methods of screening for compds. which bind to a 13C-enriched target mol., methods for calcg. the dissocn. const. of a ligand compd. which binds to a 13C-enriched target mol., and methods employed in the detn. of the specific amino acids in a 13C-enriched target mol. affected by the binding of a ligand, as well as compds. identified by these screening methods, are provided herewith.

AU Jahnke, Wolfgang; Ruedisser, Simon; Zurini, Mauro
SO Journal of the American Chemical Society (2001), 123(13), 3149-3150
CODEN: JACSAT; ISSN: 0002-7863
TI Spin label enhanced NMR screening
AB A review with refs. One of the most powerful features of biomol. NMR spectroscopy is its ability to study mol. interactions. The authors demonstrate the power of the SLAPSTIC method (spin labels attached to protein side chains as a tool to identify interacting compds.) by applying it to primary NMR screening to identify ligands for the FK506 binding protein, FKBP.7 FKBP has several lysine residues within a radius of 12-15 A from the binding site of the pipecolinic acid moiety. In conclusion, the SLAPSTIC method belongs to the most sensitive techniques of NMR screening. It offers a redn. in protein demands by 1 or 2 orders of magnitude compared to T1p relaxation expts. using nonmodified protein targets. This leads to a higher diversity of ligands to be discovered, and to a broader applicability of NMR screening.

AU Rodriguez-Mias Ricard A; Pellecchia Maurizio
SO Journal of the American Chemical Society, (2003 Mar 12) 125 (10) 2892-3.
Journal code: 7503056. ISSN: 0002-7863.
TI Use of selective Trp side chain labeling to characterize protein-protein and protein-ligand interactions by NMR spectroscopy.

AU Parker, Martin J.; Aulton-Jones, Marc; Hounslow, Andrea M.; Craven, C. Jeremy
SO Journal of the American Chemical Society (2004), 126(16), 5020-5021
CODEN: JACSAT; ISSN: 0002-7863
TI A combinatorial selective labeling method for the assignment of backbone amide NMR resonances
AB A combinatorial selective labeling (CSL) method is presented for the assignment of backbone amide NMR resonances, which has a particular application in the identification of protein-ligand interaction sites. The method builds on the dual amino acid selective labeling technique. In the CSL method a no. of different samples are produced, each with a different pattern of labeled amino acids. By analyzing peak intensities in HSQC and 2D HNCO spectra of these samples, a large no. of combinations of amino acid pairs can be simultaneously assigned. We demonstrate the method on the 27 kDa protein GFP. The samples can be produced rapidly and cost-effectively in a com. available in vitro translation system. The method greatly simplifies the process of backbone assignment and would be very straightforward to automate.

AU COCCO L; BLAKLEY R L; WALKER T E; LONDON R E
SO Biochemical and Biophysical Research Communications, (1977) Vol. 76, No. 1, pp. 183-188.
CODEN: BBRCA9. ISSN: 0006-291X.
TI A CARBON-13 NMR STUDY OF THE INTERACTION OF LIGANDS WITH ARGININE RESIDUES IN DI HYDRO FOLATE REDUCTASE.
AB 13C NMR spectra of Streptococcus faecium dihydrofolate reductase containing [13C-guanidino] arginine and ligand complexes with the labeled enzyme are reported. The spectrum of the native enzyme shows 5 well-resolved resonances (the enzyme contains 8 Arg) with a chemical shift range of 1.2 ppm. Addition of ligands to the enzyme produces distinct changes in the enzyme spectrum, and demonstrates that 13C NMR of labeled protein can be used in studies of protein-ligand interactions. An example of the use of 13C-depleted material is presented.

AU Zidek L; Stone M J; Lato S M; Pagel M D; Miao Z; Ellington A D; Novotny M V
SO Biochemistry, (1999 Aug 3) 38 (31) 9850-61.
Journal code: 0370623. ISSN: 0006-2960.
TI NMR mapping of the recombinant mouse major urinary protein I binding site occupied by the pheromone 2-sec-butyl-4,5-dihydrothiazole.
AB The interactions between the mouse major urinary protein isoform MUP-I and the pheromone 2-sec-butyl-4,5-dihydrothiazole have been characterized in solution. (15)N-labeled and (15)N, (13)C-doubly-labeled recombinant MUP-I were produced in a bacterial expression system and purified to homogeneity. Racemic 2-sec-butyl-4, 5-dihydrothiazole was produced synthetically. An equilibrium diffusion assay and NMR titration revealed that both enantiomers of the pheromone bind to the recombinant protein with a stoichiometry of 1 equiv of protein to 1 equiv of racemic pheromone. A micromolar dissociation constant and slow-exchange regime dissociation kinetics were determined for the pheromone-protein complex. (1)H, (15)N, and (13)C chemical shifts of MUP-I were assigned using triple resonance and (15)N-correlated 3D NMR experiments. Changes in protein (1)H(N) and (15)N(H) chemical shifts upon addition of pheromone were used to identify the ligand binding site. Several amide signals, corresponding to residues on one side of the binding site, were split into two peaks in the saturated protein-ligand complex. Similarly, two overlapping ligand spin systems were present in isotope-filtered NMR spectra of labeled protein bound to unlabeled pheromone. The two sets of peaks were attributed to the two possible chiralities of the pheromone. Intermolecular NOEs indicated that the orientation of the pheromone in the MUP-I binding cavity is opposite to

that modeled in a previous X-ray structure.

AU Wacks D B; Schachman H K
SO Journal of biological chemistry, (1985 Sep 25) 260 (21) 11659-62.
Journal code: 2985121R. ISSN: 0021-9258.
TI 19F nuclear magnetic resonance studies of communication between catalytic and regulatory subunits in aspartate transcarbamoylase.
AB 19F nuclear magnetic resonance (NMR) spectroscopy was used to study "communication" between the catalytic and regulatory subunits in aspartate transcarbamoylase of Escherichia coli. Hybrid enzymes composed of fluorotyrosine-labeled regulatory subunits and native catalytic subunits or of native regulatory subunits and fluorotyrosine-labeled catalytic subunits were constructed and shown to have the allosteric kinetic properties of native enzyme. These hybrids exhibited the ligand-promoted "global" conformational changes characteristic of native aspartate transcarbamoylase and alterations in the NMR spectrum when ligands bind to the active site. The NMR difference spectrum caused by the binding of the bisubstrate analog N-(phosphonacetyl)-L-aspartate to the hybrid containing 19F-labeled regulatory chains consisted of two troughs and a peak, suggesting that two tyrosines in the regulatory polypeptide chains were affected by the binding of ligand to the catalytic subunits. The increase in magnitude of the peak appeared to depend directly on the fractional saturation of the active sites. A peak with two distinct shoulders was observed in the 19F NMR spectrum of the hybrid containing fluorotyrosine in the catalytic chains when it was saturated with the ligand, whereas the spectrum for the unliganded enzyme consisted of a single peak. The NMR difference spectrum showed that the bisubstrate ligand perturbed at least two resonances, and these changes appeared to be tightly linked to the binding of the ligand.

AU Salopek-Sondi Branka; Luck Linda A
SO Protein engineering, (2002 Nov) 15 (11) 855-9.
Journal code: 8801484. ISSN: 0269-2139.
TI 19F NMR study of the leucine-specific binding protein of Escherichia coli: mutagenesis and assignment of the 5-fluorotryptophan-labeled residues.
AB The Escherichia coli L-leucine receptor is an aqueous protein and the first component in the distinct transport pathway for hydrophobic amino acids. L-leucine binding induces a conformational change, which enables the receptor to dock to the membrane components. To investigate the ligand-induced conformational change and binding properties of this protein, we used (19)F NMR to probe the four tryptophan residues located in the two lobes of the protein. The four tryptophan residues were labeled with 5-fluorotryptophan and assigned by site-directed mutagenesis. The (19)F NMR spectra of the partially ligand free proteins show broadened peaks which sharpen when L-leucine is bound, showing that the labeled wild-type protein and mutants are functional. The titration of L-phenylalanine into the 5-fluorotryptophan labeled wild-type protein shows the presence of closed and open conformers. Urea-induced denaturation studies support the NMR results that the wild-type protein binds L-phenylalanine in a different manner to L-leucine. Our studies showed that the tryptophan to phenylalanine mutations on structural units linked to the binding pocket produce subtle changes in the environment of Trp18 located directly in the binding cleft.